

Cyclopropanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, methyl ester
145348-22-7 | DTXSID60162991

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 9.14e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.83e-01

Confidence level: 3.89e-01

Nearest Neighbors from the Training Set

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Endosulfan sulfate

Measured: 1.14e-06

Predicted: 6.86e-06

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Cyclopropanecarboxylic acid, 1-
((4-chlorophenyl)sulfonyl)-,
methyl ester

Measured: 4.91e-04

Predicted: 9.14e-04

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1,2-Bis(2-
chloroethylsulfonyl)ethane

Measured: 3.56e-02

Predicted: 3.12e-02

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Chlormezanone

Measured: 9.13e-03

Predicted: 4.71e-04